

# Energy-dependent effective interactions for dilute many-body systems

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We address the issue of determining an effective two-body interaction for mean-field calculations of energies of many-body systems. We show that the effective interaction is proportional to the phase shift, and demonstrate this result in the quasiclassical approximation when there is a trapping potential in addition to the short-range interaction between a pair of particles. We calculate numerically energy levels for the case of an interaction with a short-range square-well and a harmonic trapping potential and show that the numerical results agree well with the analytical expression. We derive a generalized Gross-Pitaevskii equation which includes effective range corrections and discuss the form of the electron-atom effective interaction to be used in calculations of Rydberg atoms and molecules.

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## I. INTRODUCTION

Ultracold gases represent an ideal environment to study fundamental processes such as interparticle collisions and molecule formation. These systems are generally dilute, in the sense that the mean distance between particles  $\sim n^{-1/3}$  is typically larger than the range  $R$  of the interactions: under these conditions many-body encounters are rare, and interactions can be satisfactorily modeled by two-body collisions.

Atomic interaction potentials have a complicated structure and are generally not known exactly but, as shown by Fermi [1], the long-wavelength, low-energy properties of the two-body system can be reproduced exactly if one replaces the true potential by a suitable boundary condition for the relative wave function at the origin,

$$\psi(r) \propto 1 - \frac{a}{r}, \quad (1)$$

where  $\mathbf{r}$  is the relative coordinate vector. This boundary condition depends on a single parameter, the scattering length  $a = -\lim_{k \rightarrow 0} \delta/k$ , where  $\delta$  is the s-wave scattering phase shift. When employed in the two-body problem, this leads to an energy shift given by

$$\Delta E = \frac{2\pi\hbar^2 a}{\mu} |\psi(0)|^2, \quad (2)$$

where  $\psi(\mathbf{r})$  is the relative wave function in the absence of two-body interactions and  $\mu$  is the reduced mass of the two particles. This result leads to the interaction term in the Gross-Pitaevskii (GP) equation for the mean-field wave function of a Bose-Einstein condensed gas. The standard Fermi treatment is justified as long as the relative momentum  $k$  is so low that  $k|a| \ll 1$ , but to deal

with phenomena at higher energies the theory must be improved.

An extension of the Fermi pseudopotential was proposed in Refs. [2, 3], where the authors introduced a more general contact pseudopotential which depends on energy and which includes all partial waves  $l$ . Its s-wave component is given by

$$V_{ps}\psi = -\frac{2\pi\hbar^2}{\mu} \frac{\tan \delta}{k} \delta(\mathbf{r}) \frac{\partial r \psi}{\partial r}. \quad (3)$$

The solution of the Schrödinger equation for the pseudopotential agrees with that for the actual potential in the region where the actual potential vanishes. The magnitude of the pseudopotential is specified in terms of the tangent of the phase shift,  $\tan \delta(k)$ , where the wave number  $k$  must be taken to be that in the absence of the potential. As shown in [5, 6, 7], when the Schrödinger equation is solved for this pseudopotential one obtains eigenenergies and wave functions that reproduce very accurately the results obtained from integrating the Schrödinger equation directly for the actual microscopic potential. Following the suggestion of Ref. [8], such a pseudopotential has been employed in studies of Rydberg atoms and molecules [9, 10]. However, when used in mean-field calculations of the energy, it yields divergent energy shifts when a phase shift becomes close to  $\pi/2$  (modulo  $\pi$ ). A further proposal for the relationship between an effective interaction and the phase shift has been made in the context of deriving a generalization of the GP equation, where it has been argued that the energy shift should be proportional to the real part of the forward scattering amplitude, i.e.  $\Delta E \propto \sin \delta \cos \delta$  [11].

In this paper we explore the relationship between energy shifts and phase shifts. We shall argue that the generalization of Eq. (2) to nonzero  $k$  is to replace the scattering length by  $-\delta/k$ , a result demonstrated long ago for particles in the absence of a trapping potential [12]. In Sec. II we first demonstrate this result for two particles whose relative motion is confined to lie within a sphere, and then show that in the quasiclassical approximation it also holds if there is an additional trapping

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potential that depends on the relative coordinate. Following that we calculate numerically the energy shift for an interaction consisting of a short-range square well plus a harmonic trapping potential and show that the analytical formula fits the data well. In Sec. III, we derive a generalization of the GP equation that includes the effective range of the interaction through a derivative term and compare results with predictions based on the prescription of Ref. [11]. In Sec. IV we analyze effective interactions for ultracold Rydberg atoms and molecules. We summarize our results in Sec. V.

## II. ENERGY SHIFT

The relationship between energy shifts and phase shifts for a particle interacting with a static impurity was analyzed long ago (see e.g., [12]), and we briefly review the argument in the context of the two-particle problem. Consider two particles, with reduced mass  $\mu$ , interacting via a spherically-symmetric potential. In the absence of interaction, the relative wave function for an s-state is of the form

$$\psi(r) = A \frac{\sin(k_0 r)}{r}. \quad (4)$$

For definiteness, we imagine the relative motion to be confined by a sphere of radius  $R$ , and we impose the boundary condition that the wave function must vanish at  $r = R$ . This implies that the wave number in the absence of interaction is  $k_0 R = n\pi$ , and normalization of the wave function gives  $A = (2\pi R)^{-1/2}$ . In the presence of a short-ranged interaction  $V_{\text{sr}}(r)$ , which we shall assume vanishes more rapidly than  $r^{-1}$  for large  $r$ , the asymptotic wave function will have the same form with a phase shift:

$$\psi(r) = A \frac{\sin(kr + \delta)}{r}. \quad (5)$$

To satisfy the boundary condition at  $r = R$ , the wave number must now obey the equation  $kR + \delta = n\pi$ , which implies that the wave vector is shifted by an amount  $\Delta k = k - k_0 = -\delta/R$ . The energy shift is then given by

$$\Delta E \simeq \frac{\hbar^2}{\mu} k_0 \Delta k = \frac{2\pi\hbar^2}{\mu} \left( -\frac{\delta}{k_0} \right) |\psi(0)|^2. \quad (6)$$

Thus the energy shift due to interparticle interaction is proportional to the phase shift  $\delta$ . In the limit of zero energy, scattering theory (see e.g., [13]) shows that the s-wave phase shift is proportional to the wave vector  $\delta \simeq -ka$  and one recovers the well-known result that the effective interaction has a contact form, with strength  $U_0 = 2\pi\hbar^2 a/\mu$ .

### A. Presence of an external confining potential

One may ask whether the result (6) applies in the presence of a trapping potential. We therefore consider the same problem as above, but with an additional external potential  $V_{\text{ex}}(r)$  for the relative motion [14]. We shall assume that  $V_{\text{ex}}(r)$  increases with increasing  $r$ , and we shall impose the boundary condition that the wave function tends to zero for large  $r$ .

The basic assumption we shall make is that the trapping potential  $V_{\text{ex}}(r)$  varies negligibly over both the range  $L$  of the two-body potential  $V_{\text{sr}}(r)$  and over length scales  $\sim |\delta/k|$ , which we shall show will play the role of an energy-dependent scattering length. In addition, we assume that  $V_{\text{ex}}(r)$  varies sufficiently slowly in space and that the energy of the state is sufficiently high that we may employ the quasiclassical approximation. As usual, it is convenient to work with the quantity  $\chi = r\psi$ , and in terms of it, the Schrödinger equation becomes

$$-\frac{\hbar^2}{2\mu} \frac{d^2\chi}{dr^2} + V\chi = E\chi, \quad (7)$$

and we may take  $\chi$  to be real. The quasiclassical approximation for the potential  $V_{\text{ex}}(r)$  is

$$\psi(r) = \frac{A}{r\sqrt{p(r)}} \sin \left[ \int_0^r dr' \sqrt{\frac{2\mu[E - V_{\text{ex}}(r')]}{\hbar^2}} \right], \quad (8)$$

where  $p(r) = \sqrt{2\mu[E - V_{\text{ex}}(r)]}$  is the classical relative momentum of the two particles. The normalization constant  $A$  is fixed by requiring that the norm of  $\psi$ , i.e. the volume integral of  $|\psi|^2$  out to the classical turning point  $r = r_c$  where  $V_{\text{ex}}(r_c) = E$ , be unity. Since in Eq. (8)  $p^{-1/2}$  changes slowly over a period of oscillation of the sine function, we obtain

$$\int_0^{r_c} dr \psi^2(r) = 2\pi A^2 \int_0^{r_c} \frac{dr}{p(r)} = 1. \quad (9)$$

By choosing the zero of energy such that  $V_{\text{ex}}(0) = 0$ , the amplitude of the wave function when the positions of the two particles coincide is found to be

$$\psi(0) = \frac{\sqrt[4]{2\mu E/\hbar^4}}{\sqrt{2\pi \int_0^{r_c} dr p^{-1}(r)}}. \quad (10)$$

The phase of the semi-classical wave function obeys Bohr's quantization rule [13]

$$\int_0^{r_c} dr \sqrt{\frac{2\mu[E - V_{\text{ex}}(r)]}{\hbar^2}} = (n + \alpha)\pi, \quad (11)$$

where  $n$  is a positive integer and  $\alpha$  is a constant that depends on the nature of the potential in the vicinity of the classical turning point. The presence of the potential

$V_{\text{sr}}(r)$  induces an energy shift  $\Delta E$ , and asymptotically the wave function acquires a phase shift  $\delta$  that satisfies

$$\int_0^{r'_c} dr \sqrt{\frac{2\mu[E + \Delta E - V_{\text{ex}}(r)]}{\hbar^2}} + \delta(E + \Delta E) = (n + \alpha)\pi, \quad (12)$$

where  $r'_c$  is the appropriate classical turning point in the presence of the short-range interaction. By taking the difference between Eqs. (12) and (11), expanding the integral to first order in  $\Delta E$ , and making use of Eq. (10), one obtains the result

$$\Delta E = -\frac{2\pi\hbar^2}{\mu} \frac{\delta(E + \Delta E)}{\sqrt{2\mu E/\hbar^2}} |\psi(0)|^2, \quad (13)$$

in agreement with Eq. (6). The difference between  $r_c$  and  $r'_c$  plays no role since the integrand vanishes at the turning point.

### B. A numerical example

We now perform numerical calculations of the energy shift for a model potential. For the trapping potential, we choose a harmonic potential of frequency  $\omega$ ,  $V_{\text{ex}}(r) = \mu\omega^2 r^2/2$ , while for the particle-particle interaction we take an attractive spherically-symmetric potential which is equal to a constant,  $V_0 < 0$ , for  $r < L$  and zero otherwise. The problem is similar to that considered in Refs. [5, 6, 7], but with a simplified short-range interaction. For  $r < L$ , the solution with energy  $E$  that is regular at the origin is given by Eq. (4) with wave vector  $k = \sqrt{2\mu(E - V_0)/\hbar^2}$ ,

$$\psi_{\text{in}}(r) \propto \frac{\sin(kr)}{r}, \quad (14)$$

For  $r > L$ , the wave function is the general solution of the Schrödinger equation for the harmonic potential,

$$\psi_{\text{out}}(r) \propto e^{-r^2/2a_{\text{ho}}^2} \frac{\sqrt{\eta}}{a_{\text{ho}}} \left[ {}_1F_1\left(\frac{3-\eta}{4}, \frac{3}{2}, \frac{r^2}{a_{\text{ho}}^2}\right) - C \frac{a_{\text{ho}}}{r} {}_1F_1\left(\frac{1-\eta}{4}, \frac{1}{2}, \frac{r^2}{a_{\text{ho}}^2}\right) \right], \quad (15)$$

where  $\eta = 2E/\hbar\omega$ ,  ${}_1F_1(\alpha, \gamma, z)$  is the confluent hypergeometric function of the first kind [15] and the constant  $C = \Gamma(\frac{1-\eta}{4})/2\Gamma(\frac{3-\eta}{4})$  is chosen to ensure that  $\psi_{\text{out}}(r)$  vanishes at infinity [16, 17]. The allowed energies are found by matching at the boundary  $r = L$  the logarithmic derivatives of the solutions inside and outside the well.

The phase shift  $\delta$  for a given energy  $E$  may be found by equating at  $r = L$  the logarithmic derivatives of  $\psi_{\text{in}}$  and of the solution outside the core in the absence of the

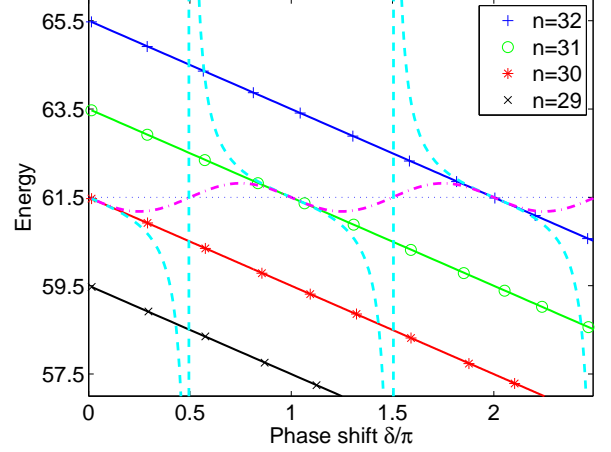


Figure 1: Energy levels for the model potential described in the text as a function of phase shift, which is given by Eq. (16). Levels are indexed by the principal quantum number  $n$ . The symbols indicate the results of numerically solving the matching condition for the Schrödinger equation at  $r = L$ . The values of the energies  $E(V_{\text{sr}}) = E(0) + \Delta E(V_{\text{sr}})$  calculated using Eq. (13) (continuous lines) are indistinguishable from the values (symbols). As a comparison, we also show the energy shifts given by Eq. (17) (dashed line) and Eq. (18) (dashed-dotted line). The energy is measured in units of  $\hbar\omega$  and the core width is  $L = 2a_{\text{ho}}$ .

smooth potential, i.e. a spherical wave with wave vector  $k_0 = \sqrt{2\mu E/\hbar^2}$ . This yields the relation

$$\delta(E) = \arctan \left[ \frac{k_0}{k} \tan(kL) \right] - k_0 L. \quad (16)$$

In Fig. 1 we show results for the energy of a few states with many nodes, obtained by direct calculation. The energy levels of our model are closely reproduced by Eq. (6), while the predictions given in Ref. [9],

$$\Delta E = -\frac{2\pi\hbar^2}{\mu} \left[ \frac{\tan \delta}{k} \right] |\psi(0)|^2, \quad (17)$$

and in Ref. [11],

$$\Delta E = -\frac{2\pi\hbar^2}{\mu} \left[ \frac{\sin \delta \cos \delta}{k} \right] |\psi(0)|^2, \quad (18)$$

are correct only for small values of  $|\delta|$  (modulo  $\pi$ ). Note that if  $|\delta| > \pi/2$  and  $|\delta/\pi - n| \ll 1$  (where  $n$  is a suitable integer), the theoretical values of the energy given by expressions (17) and (18) agree with an energy eigenvalue of the system, but one with a different number of nodes inside the short-range potential.

### III. A GENERALIZED GROSS-PITAEVSKII EQUATION

In the numerical example above, we considered a state with many nodes. For applications to Bose-Einstein condensates, the relevant wave numbers are usually small, and therefore it is interesting to look at the opposite case of small but nonzero wave numbers. When the Wigner threshold condition  $k|a| \ll 1$  is violated, the s-wave phase shift is no longer linear in the wave vector, and its energy dependence can be written for potentials that fall off more rapidly than  $r^{-5}$  for large  $r$  as

$$k \cot \delta = -\frac{1}{a} + \frac{1}{2}r_e k^2 + o(k^2), \quad (19)$$

where  $r_e$  is the effective range of the interaction [18]. For small phase shifts  $\delta \simeq \tan \delta - \tan^3 \delta / 3$  and we find:

$$-\frac{\delta}{k} = a(1 - g_2 k^2) \quad (20)$$

where we have introduced

$$g_2 = \frac{a^2}{3} - \frac{ar_e}{2}. \quad (21)$$

The energy shift is then given by

$$\Delta E = \frac{2\pi\hbar^2 a}{\mu} [1 - g_2 k^2] |\psi(0)|^2. \quad (22)$$

It is interesting to note that in the case of hard spheres of diameter  $a$  the boundary condition on the surface of the sphere implies that  $\delta = -ka$  for all  $k$  and therefore  $g_2$  (and all higher terms in an expansion of  $\delta$  in powers of  $k$ ) should vanish. Since from Eq. (19)  $r_e = 2a/3$  for the hard-sphere potential, one indeed finds  $g_2 = 0$  from Eq. (21). Our result is to be contrasted with the expression  $g_2 = a^2 - ar_e/2$  based on the approximation (18) for the interaction energy [11].

As shown in Ref. [11], the energy shift can be inserted into the energy functional to obtain a generalization of the GP equation for the condensate wave function  $\Psi$  that contains a derivative term in the interaction energy:

$$i\hbar \frac{\partial}{\partial t} \Psi = \left[ -\frac{\hbar^2}{2m} \nabla^2 + V(r) + U_0 \left( |\Psi|^2 + g_2 \nabla^2 |\Psi|^2 \right) \right] \Psi. \quad (23)$$

Contributions from higher partial waves may be included through the addition of higher derivative terms, as described for Fermi systems in Ref. [4].

To test the validity of this prediction, we have performed numerical integrations of the relative motion for the two-body problem considered above, with a harmonic trapping potential and a short-range square well potential, but for the lowest state rather than the excited states considered in Sec. II. The results are compared with those obtained from analytical approximations. Figure 2 shows that the inclusion of the effective range correction with  $g_2$  given by Eq. (21) greatly improves the prediction given by the simple scattering length approximation as soon as the condition  $k|a| \ll 1$  is violated.

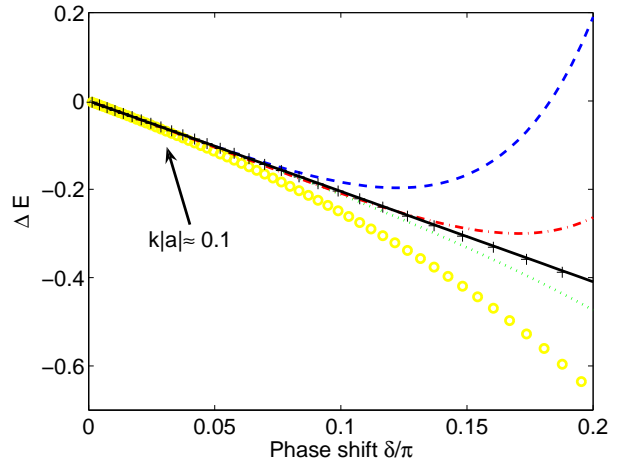


Figure 2: Energy shift for the ground state ( $n = 0$ ) of the combined potential discussed in the text. The exact results (crosses) are compared with the energy shifts given by the formula  $\Delta E = 2\pi\hbar^2 f |\psi(0)|^2 / \mu$ , where  $f = a$  (circles),  $f = -\tan \delta / k$  (dotted line),  $f = -\delta / k$  (solid line), by the result that includes the effective range correction,  $f = a(1 - g_2 k^2)$  (dashed-dotted line), and by the result of Ref. [11],  $f = a(1 - \tilde{g}_2 k^2)$  (dashed line). The energy is measured in units of  $\hbar\omega$  and the core width is  $L = 0.25a_{\text{ho}}$ .

### IV. APPLICATION TO RYDBERG MOLECULES

In Rydberg atoms the valence electron is in a highly excited state with principal quantum number  $n \gtrsim 20$ , and within quantum defect theory it is described in terms of generalized hydrogenic wave functions. By analogy with the structures created around positive ions in liquid helium [20] or BECs [21, 22], a Rydberg atom with a large electric dipole moment inside a BEC may create remarkable deformations of the condensate density in its surroundings. The additional degree of freedom introduced by the permanent electric dipole moment could also be used to realize conditional logic gates for quantum information processing [23].

On the experimental side, Rydberg atoms have already been created in an ultracold environment [24], and there is a proposal to excite and trap single Rydberg atoms inside a BEC [25]. Being overall electrically neutral, Rydberg atoms are not accelerated by the stray electric fields which are unavoidable in experimental vacuum chambers. This is particularly relevant since, in a typical apparatus for ultracold atoms, stray fields would drag an ion outside the condensate in a time much less than 1 ms, making difficult the observation of the induced density disturbances.

In recent work [9, 10], it has been predicted that the tailored excitation of single atoms in a BEC towards a Rydberg state would induce the formation of molecules characterized by ultra-long ranges ( $R \sim 2000$  a.u.) and very large permanent electric dipole moments. In these

papers, the s-wave molecular potential between a ground state atom and a Rydberg atom was taken to be

$$V_s(\vec{r}, \vec{R}) = -\frac{2\pi\hbar^2}{\mu} \frac{\tan \delta_0[k(R)]}{k} \delta(\vec{r} - \vec{R}), \quad (24)$$

where  $\vec{r}$  and  $\vec{R}$  are the positions of the electron and of the ground state atom relative to the Rydberg ion,  $\delta_0[k(R)]$  is the energy-dependent phase shift and the electron wave number  $k(R)$  is given by the hydrogenic relation  $k^2(R)/2 - 1/R = -1/2n^2$ . The authors of [9, 10] follow Omont [8] and conclude that the appropriate potential for the excited electron is given, in the Born-Oppenheimer approximation, by

$$U_s(\vec{R}) = E_{nl} - \frac{2\pi\hbar^2}{\mu} \frac{\tan \delta_0[k(R)]}{k} |\psi_{nl0}(\vec{R})|^2, \quad (25)$$

where  $E_{nl}$  and  $\psi_{nl0}$  are the unperturbed atomic Rydberg energy and wave function (with quantum numbers  $n \sim 30$ ,  $l \lesssim 2$  and  $m = 0$ ). As discussed above, while the potential in Eq. (24) reproduces accurately eigenenergies and wave functions of the Schrödinger equation, it should not be used in mean-field calculations, where it yields unphysical divergent energy shifts in the presence of a resonance.

This issue is particularly relevant for the scattering in the p-wave channel, where the e-Rb(5s) scattering phase shift  $\delta_{l=1}$  has a resonance at an energy of approximately 30 meV, corresponding to a distance between the Rb ion and the ground state atom of about 700 a.u.: here Omont's expression for the energy shift  $\Delta E(\vec{R}) \propto |\vec{\nabla} \psi_{nl0}(\vec{R})|^2 \tan \delta_1(k)/k^3$  diverges. However, according to the arguments we have given, the appropriate effective interaction for a mean-field calculation is not given by this expression, but rather by one with the tangent of the phase shift replaced by the phase shift itself, and consequently there are no divergence problems.

## V. CONCLUSION

In this paper we have studied the expression for the effective two-body interaction to be used in mean-field

calculations of the energy of a state. All results agree in the limit of zero energy, but there are differences at higher energies. We have argued that the appropriate effective interaction is proportional to the phase shift, rather than other expressions that have been suggested, and we show that this holds analytically for the states of two particles in a trap in the quasiclassical approximation. We have calculated energy levels numerically for the problem of two particles interacting via a short-range square-well potential in the presence of a harmonic confining potential and have demonstrated that the analytical expression in terms of the phase shift agrees well with the numerical data, both for the ground state and for excited states with many nodes. Since an effective interaction proportional to  $\tan \delta$  gives the correct wave functions and energy eigenvalues when inserted in the Schrödinger equation, our results show that the choice of effective interaction depends on the application.

In this article, we have also considered corrections to the Gross-Pitaevskii equation to allow for the nonzero energy of the relative motion of two particles and have derived a generalized Gross-Pitaevskii equation that takes into account the effective range. This equation gives a better approximation to the numerical results for energy eigenvalues than does an earlier proposal [11]. A problem for future work is to include contributions from higher partial waves in the GP equation. Finally, we have argued that the effective two-body interaction to be used in calculations of Rydberg atoms and molecules should be taken to be proportional to the phase shift.

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$$k \cot \delta = -\frac{1}{a} + \frac{\pi\beta_4^2}{3a^2}k + Ak^2 \ln(k\beta_4) + Bk^2 + o(k^2),$$
 where  $\beta_4$ ,  $A$  and  $B$  are constants with dimensions of a length.
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